9-Propyl-beta-carboline

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.63

Global applicability domain: Inside

Local applicability domain index: 9.69e-01

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

Image not found
1,2,4-Trichlorodibenzo-1,4-dioxin
Measured: 8.97
Predicted: 8.77

Image not found
4,4'-Dibromodiphenyl ether
Measured: 8.64
Predicted: 8.53